Temple University

Statistical Science & Data Analytics

The Eigenvectors & Eigenvalues of Principal Component Analysis

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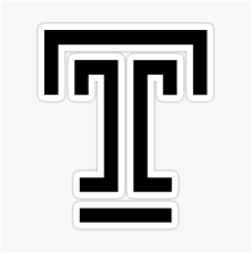

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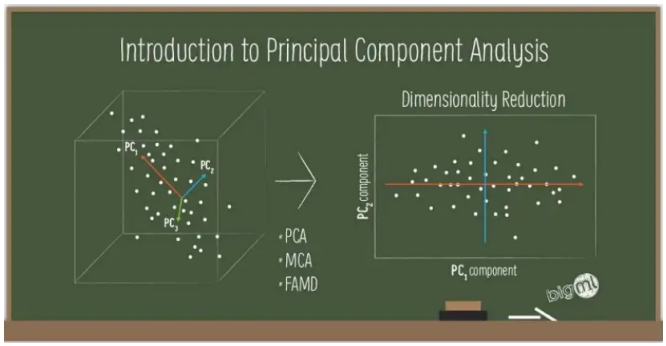


[2]

Figure 1: *Right: variance maximized 3d data projected into 2d*

1 Introduction

Principal component analysis is a statistical technique that is used to reduce the dimensionality of large data sets. It was first mentioned in a paper written by a famous statistician named Karl Pearson in 1901, who once described the technique as quote, "finding lines and planes of closest fit to systems of points in space".[1] In this paper I will only be discussing the mathematical core of PCA, which allows us to find these lines and planes of best fit.

2 Understanding Principal Component Analysis

Even if one understands statistics, understanding principal component analysis could be a challenge. So, in this section I will try to simplify what PCA is as much as I can.

In the world of data, "features" is just another term for the variables you find in a dataset. More succinctly, we can think of them as the columns of a dataset. Features come in different types. Some are "discrete," meaning they take on specific, separate values. For example, imagine counting the number of cars passing a particular spot on the road at a given time. On the other hand, some features are "continuous," meaning they can take on any value within a range. The salary of a person or the amount of income tax they pay annually are good examples of what continuous features are. They're not limited to specific, separate numbers but can vary more fluidly.

When an analyst builds a model like a multiple linear regression, they would use continuous features. Think of each "feature"as holding a bit of information that is special and unique. This is also known as the variance of that feature. In multiple linear regression, the variation or "spread" within these features is crucial because it helps us understand how much each feature tells us about what we're trying to predict, which is often called the dependent variable or "Y-variable."

But what happens when we have an abundance of features? It becomes essential to figure out which ones really matter. The goal is to keep all the useful variation that helps our model but disregard the features that don't add any value. This is where Principal Component Analysis (PCA) comes into play. PCA helps by distilling the data to retain only the most impactful features, ensuring our model remains powerful without being congested with unnecessary information.

In its essence, PCA boils down to creating a new set of features, called principal components. Imagine you have a dataset with many columns; PCA transforms these into a new set of columns. Each of these new columns is a principal component and represents a linear combination of the originals.

Think of principal components as ingredients in a recipe, where each ingredient (or principal component) is a mix of the original variables. The magic of PCA is that it arranges these ingredients in a very specific order: the first principal component captures the most variance (or information) from the data, the second captures the next most, and so on. The goal is to pack as much information as possible into the first few principal components (usually the first three).

To visualize how much information each principal component holds, we use something called a scree plot. This plot shows us the percentage of variance each principal component captures from the data. With this, analysts can decide which components to keep — typically those that hold the most information — and which ones to discard, making the data more manageable and focused on the most meaningful aspects.

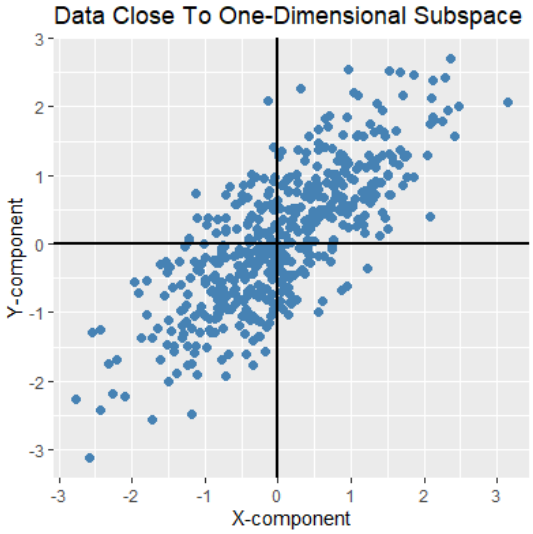


Figure 2: *2-dimensional data that is close to a 1-dimensional subspace we can call C*

In the above diagram, we can see a data set that represents the relationship between two features with data points that cut through the origin. What if we could preserve all of the useful variance contained within our two features and then reduce the set of features by projecting the two dimensional dataset onto a one dimensional line? This is exactly what PCA does.

Given the low dimensionality of our example data set, this idea might not seem too useful. However, what if we had a 50-dimensional data set (a dataset with 50 features)? This is where PCA shines. It allows the analyst to make their data set less crowded with redundant information while preserving most of the useful information. With that being said, the question remains, how can we fit higher dimensional sub-spaces to lower dimensional sub-spaces using linear algebra?

3 Subspace Fitting: Centered Data

Given that PCA appears to be overall complex, the mathematical procedure to derive the principal components is straightforward. The task of finding principal components is a bit easier if our data is centered and already passes through the origin like the two dimensional dataset above.

In this example, we are going to find the 1-dimensional subspace that best approximates data set A. We will also find the total squared distance of the data points to the subspace we fit. This may seem much like linear curve fitting, however, it is slightly different. Subspace fitting minimizes the orthogonal distances from each data point to the line (eigenvector), whereas, linear curve fitting minimizes the vertical distances from each data point to the line.

3.1 Finding Eigenvalues & Eigenvectors: Centered 2-Dimensional Data

First we calculate A^TA to get our symmetric matrix, find $det(A-\lambda I)$ and $p_A(\lambda)$, then, derive the roots from $p_A(\lambda)$, the characteristic polynomial. This will yield the eigenvalues. We will then plug in the eigenvalues into $A-\lambda I$ to derive a corresponding eigenspace for every eigenvector that we find. The result will be each eigenvector and eigenvalue of the symmetric matrix. *Consider the following collection of points in* $\mathbb{R}^2$.[6]

$$A = \left\{ \begin{bmatrix} 1 \\ -1 \end{bmatrix}, \begin{bmatrix} -2 \\ 1 \end{bmatrix}, \begin{bmatrix} 3 \\ -2 \end{bmatrix}, \begin{bmatrix} 2 \\ -2 \end{bmatrix}, \begin{bmatrix} -2 \\ 1 \end{bmatrix}, \begin{bmatrix} 3 \\ -1 \end{bmatrix}, \begin{bmatrix} -3 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 3 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ -2 \end{bmatrix} \right\}$$

$$A = \begin{bmatrix} 1 & -2 & 3 & 2 & -2 & 3 & -3 & 0 & 0 & 0 \\ -1 & 1 & -2 & -2 & 1 & -1 & 0 & 3 & 0 & -2 \end{bmatrix}$$

$$B = A^TA = \begin{bmatrix} 40 & -18 \\ -18 & 25 \end{bmatrix}$$

$$det(B-\lambda_n I) = \begin{bmatrix} 40-\lambda_n & -18 \\ -18 & 25-\lambda_n \end{bmatrix}$$

$$\begin{aligned} p_B(\lambda) &= (40-\lambda)(25-\lambda) - (-18)(-18) \\ &= \lambda^2 - 65\lambda + 676 \end{aligned}$$

$$\lambda_1 = \frac{-(-65) + \sqrt{(-65^2) - 4(1)(676)}}{2(1)} = 52$$

$$\lambda_2 = \frac{-(-65) - \sqrt{(-65^2) - 4(1)(676)}}{2(1)} = 13$$

$$\bar{v}_1 = \begin{bmatrix} -\frac{3}{2} \\ 1 \end{bmatrix} \qquad \bar{v}_2 = \begin{bmatrix} \frac{2}{3} \\ 1 \end{bmatrix}$$

As we can see, we have two eigenvalues $\{\lambda_1, \lambda_2\}$ and two eigenvectors $\{\bar{v}_1, \bar{v}_2\}$. If we pick the largest eigenvalue, $\lambda_1 = 52$, and its corresponding eigenvector $\bar{v}_1 = (-\frac{3}{2}, 1)$, this is the closest 1-dimensional subspace that is spanned by $\{\bar{v}\}$. In other words, the first eigenvector points to the direction in space in which the data has the largest variance. It essentially tells us how to reorient the initial $\{x, y\}$ axes, such that we get the best maximized variance view of the data.

3.2 Finding Eigenvalues & Eigenvectors: Centered 3-Dimensional Data

To further demonstrate the finding of lower dimensional sub-spaces, we once again are going to follow the previous procedure. But instead of just finding the closest 1-dimensional subspace, we will find the closest 2-dimensional subspace, as well as, the closest 3-dimensional subspace. One subspace for each dimension. *Consider the following collection of points in* $\mathbb{R}^3$.[6]

$$A = \left\{ \begin{bmatrix} 0 \\ 0 \\ 9 \end{bmatrix}, \begin{bmatrix} 1 \\ 0 \\ -3 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}, \begin{bmatrix} 0 \\ 5 \\ -4 \end{bmatrix}, \begin{bmatrix} 6 \\ -2 \\ 13 \end{bmatrix}, \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 2 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 1 \end{bmatrix}, \begin{bmatrix} 2 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 4 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 \\ -3 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 4 \end{bmatrix} \right\}$$

$$A = \begin{bmatrix} 0 & 1 & 0 & 0 & 6 & 1 & 0 & 0 & 2 & 4 & 1 & 0 \\ 0 & 0 & 0 & 5 & -2 & 0 & 2 & 1 & 0 & 0 & -3 & 0 \\ 9 & -3 & 1 & -4 & 13 & 0 & 0 & 1 & 0 & 0 & 0 & 4 \end{bmatrix}$$

$$B = A^T A = \begin{bmatrix} 59 & -15 & 75 \\ -15 & 43 & -45 \\ 75 & -45 & 293 \end{bmatrix}$$

$$det(B - \lambda_n I) = \begin{bmatrix} 59 - \lambda_n & -15 & 75 \\ -15 & 43 - \lambda_n & -45 \\ 75 & -45 & 293 - \lambda_n \end{bmatrix}$$

$$p_B(\lambda) = -\lambda^3 - 395\lambda^2 + 24548\lambda - 417316$$

$$= -(\lambda - 323)(\lambda - 38)(\lambda - 34)$$

$$\lambda_1 = 323 \;\; \lambda_2 = 38 \;\; \lambda_3 = 34$$

$$\bar{v}_1 = \begin{bmatrix} -\frac{5}{17} \\ \frac{3}{17} \\ 1 \end{bmatrix} \qquad \bar{v}_2 = \begin{bmatrix} -\frac{5}{2} \\ \frac{3}{2} \\ 1 \end{bmatrix} \qquad \bar{v}_2 = \begin{bmatrix} \frac{3}{5} \\ 1 \\ 0 \end{bmatrix}$$

3.3 Sum of Squared Distances to a Subspace: Centered 3-Dimensional Data

Now that we have our eigenvalues $\{\lambda_1, \lambda_2, \lambda_3\}$ in decreasing order, along with the associated eigenvectors $\{\bar{v}_1, \bar{v}_2, \bar{v}_3\}$, we can find the closest subspaces in $\{\mathbb{R}, \mathbb{R}^2, \mathbb{R}^3\}$. The closest 1-dimensional subspace is spanned by the eigenvector associated with the largest eigenvalue $\{\bar{v}_1\}$. The closest 2-dimensional subspace is spanned by the eigenvectors associated with the first and second largest eigenvalues $\{\bar{v}_1, \bar{v}_2\}$, and the closest 3-dimensional subspace is spanned by all three eigenvectors $\{\bar{v}_1, \bar{v}_2, \bar{v}_3\}$. Furthermore, we have the total squared distances to each respective subspace.

$$SSd_{\mathbb{R}} = \lambda_2 + \lambda_3 = 323 + 38 = 361$$

$$SSd_{\mathbb{R}^2} = \lambda_3 = 34$$

$$SSd_{\mathbb{R}^3} = 0 \quad \text{since all data points lie in } \mathbb{R}^3$$

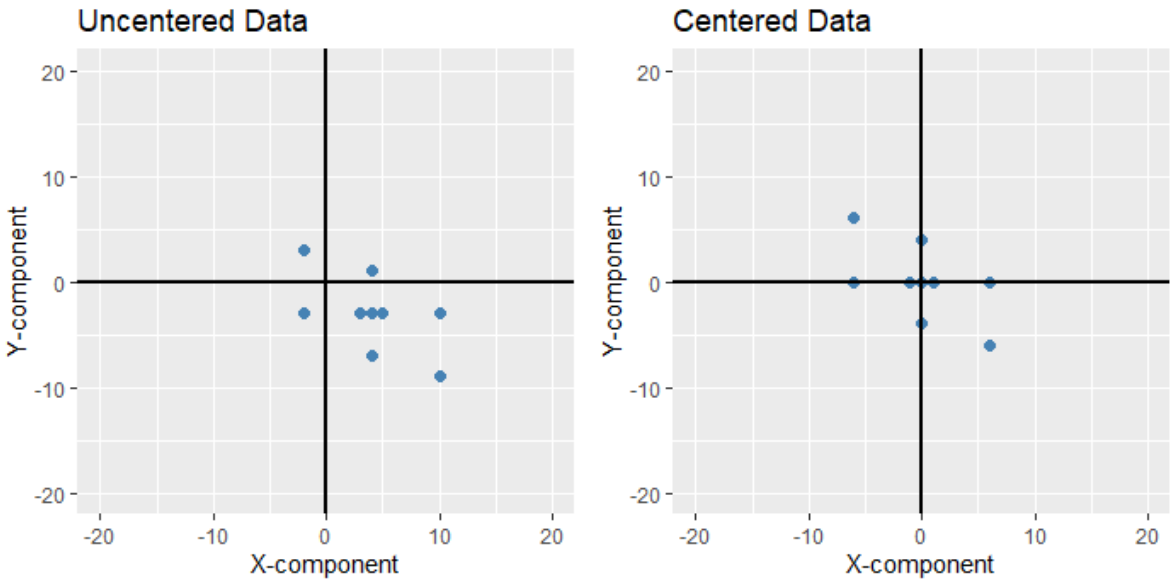


Figure 3: *Left: un-centered data in a 2-dimensional subspace that is close to a 1-dimensional subspace. Right: data after we subtract the mean from every vector in the data set.*

4 Affine Subspace Fitting: Uncentered Data

The above examples are an ideal scenario regarding fitting high dimensional data to lower dimensional subspaces. Most of the time, the data that we gather will not be as cooperative. This is where the affine sub-space fitting problem comes in. The procedure is about the same as in the examples above, however, there is an additional step. We must compute the centroid of the data first. The centroid is the vector for which $\bar{y}$ and $\bar{x}$ are equal to one another. Once we calculate the centroid, we can subtract it from our set of vectors. The resulting set of data points will then be centered around the origin (0, 0). Note, this does nothing to change the position of the data points relative to one another. It only shifts the data so that it is mathematically centered about the origin.

In the next example, I will compute the centroid and find the 1-dimensional affine subspace that best approximates this collection of points. The last step will be to find the total squared distance of the points to the subspace. *Consider the following collection of points in* $\mathbb{R}^2$. [6]

$$A = \left\{ \begin{bmatrix} 4 \\ -3 \end{bmatrix}, \begin{bmatrix} 10 \\ -9 \end{bmatrix}, \begin{bmatrix} 4 \\ -7 \end{bmatrix}, \begin{bmatrix} -2 \\ 3 \end{bmatrix}, \begin{bmatrix} 10 \\ -3 \end{bmatrix}, \begin{bmatrix} 4 \\ -3 \end{bmatrix}, \begin{bmatrix} 5 \\ -3 \end{bmatrix}, \begin{bmatrix} 4 \\ 1 \end{bmatrix}, \begin{bmatrix} -2 \\ -3 \end{bmatrix}, \begin{bmatrix} 3 \\ -3 \end{bmatrix} \right\}$$

4.1 Compute Centroid & Center Data: Uncentered 2-Dimensional Data

$$B = \frac{1}{10}\left\{\begin{bmatrix}4\\-3\end{bmatrix} + \begin{bmatrix}10\\-9\end{bmatrix} + \begin{bmatrix}4\\-7\end{bmatrix} + \begin{bmatrix}-2\\3\end{bmatrix} + \begin{bmatrix}10\\-3\end{bmatrix} + \begin{bmatrix}4\\-3\end{bmatrix} + \begin{bmatrix}5\\-3\end{bmatrix} + \begin{bmatrix}4\\1\end{bmatrix} + \begin{bmatrix}-2\\-3\end{bmatrix} + \begin{bmatrix}3\\-3\end{bmatrix}\right\}$$

$$= \frac{1}{10}\begin{bmatrix}40\\-30\end{bmatrix} = \begin{bmatrix}4\\-3\end{bmatrix}$$

$$C = A - B = \left\{\begin{bmatrix}0\\0\end{bmatrix}, \begin{bmatrix}-6\\6\end{bmatrix}, \begin{bmatrix}0\\4\end{bmatrix}, \begin{bmatrix}6\\-6\end{bmatrix}, \begin{bmatrix}-6\\0\end{bmatrix}, \begin{bmatrix}0\\0\end{bmatrix}, \begin{bmatrix}-1\\0\end{bmatrix}, \begin{bmatrix}0\\-4\end{bmatrix}, \begin{bmatrix}6\\0\end{bmatrix}, \begin{bmatrix}1\\0\end{bmatrix}\right\}$$

4.2 Eigenvalues & Eigenvectors: Uncentered 2-Dimensional Data

$$C = \begin{bmatrix}0 & -6 & 0 & 6 & -6 & 0 & -1 & 0 & 6 & 1\\ 0 & 6 & 4 & -6 & 0 & 0 & 0 & -4 & 0 & 0\end{bmatrix}$$

$$D = C^T C = \begin{bmatrix}146 & -72\\ -72 & 104\end{bmatrix}$$

$$det(D - \lambda_n I) = \begin{bmatrix}146 - \lambda_n & -72\\ -72 & 104 - \lambda_n\end{bmatrix}$$

$$p_D(\lambda) = \lambda^2 - 250\lambda + 10000$$

$$\lambda_1 = \frac{-(-250) + \sqrt{(-250^2) - 4(1)(10000)}}{2(1)} = 200$$

$$\lambda_2 = \frac{-(-250) - \sqrt{(-250^2) - 4(1)(10000)}}{2(1)} = 50$$

$$\bar{v}_1 = \begin{bmatrix}-\frac{4}{3}\\1\end{bmatrix} \qquad \bar{v}_2 = \begin{bmatrix}\frac{3}{4}\\1\end{bmatrix}$$

$$W = B + C = \{b + c \mid c \in C\} = \left\{\begin{bmatrix}4\\-3\end{bmatrix} + y\begin{bmatrix}-\frac{4}{3}\\1\end{bmatrix} \mid y \in \mathbb{R}\right\} \in \mathbb{R}$$

Now that we have both our eigenvectors and their associated values we can find the closest 1-dimensional subspace as well as the sum of the squared distances from it. Remember, when reducing 2-dimensions to 1-dimension the desired subspace W is spanned by the eigenvector with the largest eigenvalue. The total squared distance is the λ_2.

$$SSd_{\mathbb{R}} = \lambda_2 = 50$$

$$SSd_{\mathbb{R}^2} = 0 \quad \text{since all data points lie in } \mathbb{R}^2$$

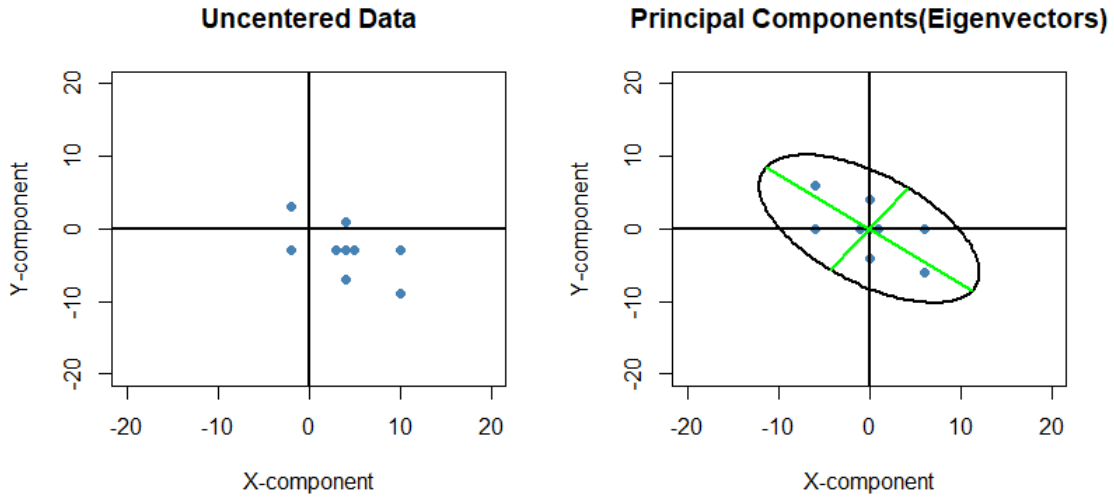


Figure 4: *Left: uncentered data Right: centered data with principal components overlaid.The orthogonal eigenvectors span the direction of greatest variance*

4.3 Tying it All Together

For our final example, we will use three dimensional data to tie all of the concepts together into a complete analysis. We will first visualize our data in three dimensions, compute the centroid, compute our nxn symmetric matrix, then find the closest 1 and 2 dimensional affine subspaces that minimizes the square distances from our data to the subspace. *Consider the following collection of points in* $\mathbb{R}^3$. [6]

$$A = \left\{ \begin{bmatrix} 0 \\ -2 \\ 2 \end{bmatrix}, \begin{bmatrix} 6 \\ 2 \\ 2 \end{bmatrix}, \begin{bmatrix} 2 \\ 2 \\ 6 \end{bmatrix}, \begin{bmatrix} 3 \\ 2 \\ 2 \end{bmatrix}, \begin{bmatrix} 3 \\ 0 \\ 5 \end{bmatrix}, \begin{bmatrix} 5 \\ 0 \\ 2 \end{bmatrix}, \begin{bmatrix} 4 \\ -2 \\ -2 \end{bmatrix}, \begin{bmatrix} 5 \\ 0 \\ 2 \end{bmatrix}, \begin{bmatrix} 1 \\ 0 \\ 2 \end{bmatrix}, \begin{bmatrix} 3 \\ 0 \\ -1 \end{bmatrix}, \begin{bmatrix} 3 \\ 0 \\ 1 \end{bmatrix}, \begin{bmatrix} 3 \\ 0 \\ 3 \end{bmatrix}, \begin{bmatrix} 1 \\ 0 \\ 2 \end{bmatrix}, \begin{bmatrix} 3 \\ -2 \\ 2 \end{bmatrix} \right\}$$

4.4 Compute Centroid & Center Data: Uncentered 3-Dimensional Data

$$B = \frac{1}{14}\left\{\begin{bmatrix}0\\-2\\2\end{bmatrix} + \begin{bmatrix}6\\2\\2\end{bmatrix} + \begin{bmatrix}2\\2\\6\end{bmatrix} + \begin{bmatrix}3\\2\\2\end{bmatrix} + \begin{bmatrix}3\\0\\5\end{bmatrix} + \begin{bmatrix}5\\0\\2\end{bmatrix} + \begin{bmatrix}4\\-2\\-2\end{bmatrix} + \begin{bmatrix}5\\0\\2\end{bmatrix} + \begin{bmatrix}1\\0\\2\end{bmatrix} + \begin{bmatrix}3\\0\\-1\end{bmatrix} + \begin{bmatrix}3\\0\\1\end{bmatrix} + \begin{bmatrix}3\\0\\3\end{bmatrix} + \begin{bmatrix}1\\0\\2\end{bmatrix} + \begin{bmatrix}3\\-2\\2\end{bmatrix}\right\}$$

$$= \frac{1}{14}\begin{bmatrix}42\\0\\28\end{bmatrix} = \begin{bmatrix}3\\0\\2\end{bmatrix}$$

$$C = A - B = \left\{\begin{bmatrix}-3\\-2\\0\end{bmatrix}, \begin{bmatrix}3\\2\\0\end{bmatrix}, \begin{bmatrix}-1\\2\\4\end{bmatrix}, \begin{bmatrix}0\\2\\0\end{bmatrix}, \begin{bmatrix}0\\0\\3\end{bmatrix}, \begin{bmatrix}2\\0\\0\end{bmatrix}, \begin{bmatrix}1\\-2\\-4\end{bmatrix}, \begin{bmatrix}2\\0\\0\end{bmatrix}, \begin{bmatrix}-2\\0\\0\end{bmatrix}, \begin{bmatrix}0\\0\\-3\end{bmatrix}, \begin{bmatrix}0\\0\\-1\end{bmatrix}, \begin{bmatrix}0\\0\\1\end{bmatrix}, \begin{bmatrix}-2\\0\\0\end{bmatrix}, \begin{bmatrix}0\\-2\\0\end{bmatrix}\right\}$$

$$C = \begin{bmatrix} -3 & 3 & -1 & 0 & 0 & 2 & 1 & 2 & -2 & 0 & 0 & 0 & -2 & 0 \\ -2 & 2 & 2 & 2 & 0 & 0 & -2 & 0 & 0 & 0 & 0 & 0 & 0 & -2 \\ 0 & 0 & 4 & 0 & 3 & 0 & -4 & 0 & 0 & -3 & -1 & 1 & 0 & 0 \end{bmatrix}$$

4.5 Eigenvalues & Eigenvectors: Uncentered 3-Dimensional Data

$$D = C^T C = \begin{bmatrix} 36 & 8 & -8 \\ 8 & 24 & 16 \\ -8 & 16 & 52 \end{bmatrix}$$

$$det(D - \lambda_n I) = \begin{bmatrix} 36-\lambda_n & 8 & -8 \\ 8 & 24-\lambda_n & 16 \\ -8 & 16 & 52-\lambda_n \end{bmatrix}$$

$$p_D(\lambda) = -\lambda^3 + 112\lambda^2 - 3600\lambda - 28800$$

$$= -(\lambda - 12)(\lambda - 40)(\lambda - 60)$$

$$\lambda_1 = 12 \;\; \lambda_2 = 40 \;\; \lambda_3 = 60$$

$$\bar{v}_1 = \begin{bmatrix}1\\-2\\1\end{bmatrix} \qquad \bar{v}_2 = \begin{bmatrix}2\\1\\0\end{bmatrix} \qquad \bar{v}_3 = \begin{bmatrix}-\frac{1}{5}\\\frac{2}{5}\\1\end{bmatrix}$$

4.6 Sum of Squared Distance to $\mathbb{R}^n$: Uncentered 3-Dimensional Data

$$SSd_{\mathbb{R}} = \lambda_2 + \lambda_3 = 40 + 60 = 100$$

$$SSd_{\mathbb{R}^2} = \lambda_3 = 60$$

$$SSd_{\mathbb{R}^3} = 0 \quad \text{since all data points lie in } \mathbb{R}^3$$

4.7 Closest One, Two, & Three Dimensional Subspaces

$$W_1 = B + C = \{b + c \mid c \in C\} = \left\{ \begin{bmatrix} 3 \\ 0 \\ 2 \end{bmatrix} + x \begin{bmatrix} 1 \\ -2 \\ 1 \end{bmatrix} \mid x \in \mathbb{R} \right\} \in \mathbb{R}$$

$$W_2 = B + C = \{b + c \mid c \in C\} = \left\{ \begin{bmatrix} 3 \\ 0 \\ 2 \end{bmatrix} + \left\{ x \begin{bmatrix} 1 \\ -2 \\ 1 \end{bmatrix} + y \begin{bmatrix} 2 \\ 1 \\ 0 \end{bmatrix} \right\} \mid x, y \in \mathbb{R} \right\} \in \mathbb{R}^2$$

$$W_3 = B + C = \{b + c \mid c \in C\} = \left\{ \begin{bmatrix} 3 \\ 0 \\ 2 \end{bmatrix} + \left\{ x \begin{bmatrix} 1 \\ -2 \\ 1 \end{bmatrix} + y \begin{bmatrix} 2 \\ 1 \\ 0 \end{bmatrix} + z \begin{bmatrix} -\frac{1}{5} \\ \frac{2}{5} \\ 1 \end{bmatrix} \right\} \mid x, y, z \in \mathbb{R} \right\} \in \mathbb{R}^3$$

5 Scree Plot

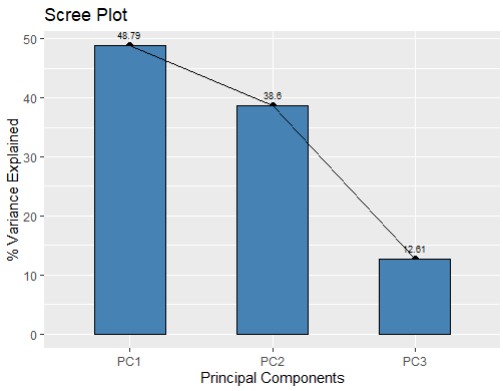
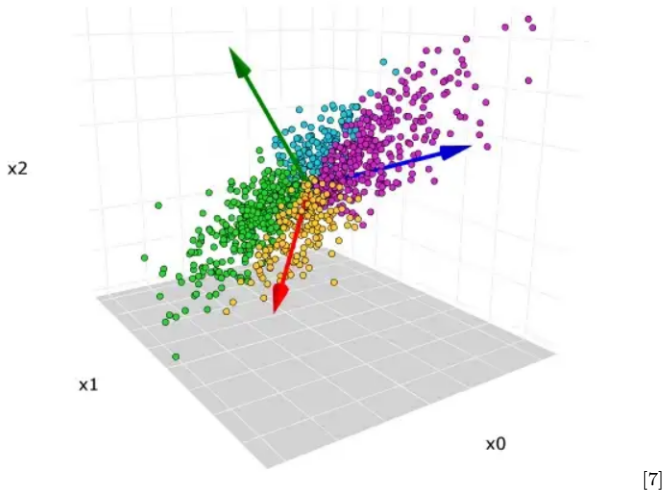


Figure 5: *a scree plot that summarizes the percentage of explained variance by each eigenvector*

5.1 What is a Scree Plot?

A scree plot is a useful tool when performing PCA. It summarizes how much variance is explained by our principal components, otherwise known as, the eigenvectors. After running the data in section 4.3 through a PCA analysis in R, I created this scree plot to summarize how much information is explained by each principal component. As we can see, PC1's direction contains the most variance at 49%, whereas, PC2's direction contains 39% ,the second most, and PC3's direction contains the least at 13%. If I were an analyst looking to build a model with these results I would most certainly want to try to include all of these components. This is because three features is not a lot when it comes to model building. Disregarding 12% of the variance when the number of features is so little can be disastrous and can lead to inaccurate results. Like stated in section two, PCA really shines when there is 5 or more features.

6 Conclusion



[7]

Figure 6: *centered 3-dimensional data that is close to a 2-dimensional subspace with associated eigenvectors*

In conclusion, principal component analysis can be defined as an orthogonal linear transformation that transforms the data to a new coordinate system such that the greatest variance by some scaler projection of the data comes to lie on the first component, the second greatest on the second component, and so on.[8]

In other words, PCA finds the lines of best fit, rotates the eigenvectors and transforms the data, such that, the shadows, or images of the data, in the nth dimension, get projected down into lower dimensions. You can think of it as trying to figure out which direction you should view your data so that the distance between each data point is maximized.

It will generally be the case in PCA, that the number of principal components is equal to the number of eigenvalues. Once we find our eigenvectors we rotate them such that they become our new axes through which we view the variance maximized data. One eigenvector for every feature. The best part of this dimensionality reduction technique is that it will generally be the case that only the first few principal components will be referenced in our final analysis.

References

[1] Pearson, K. (1901). "On Lines and Planes of Closest Fit to Systems of Points in Space". Philosophical Magazine. 2 (11): 559–572. doi:10.1080/14786440109462720.

[2] Guide to principal component analysis. (n.d.). https://medium.com/analytics-vidhya/guide-to-principal-component-analysis-ab04a8a9c305

[3] Kumar, R. (2018, June 19). Understanding Principal Component Analysis - Rishav Kumar. *Medium*. URL:https://medium.com/@aptrishu/understanding-principle-component-analysis-e32be0253ef0 Retrieved. December 2022

[4] StatQuest with Josh Starmer. (2018, April 2). *StatQuest: Principal Component Analysis*(PCA), *Step-by-Step* [Video]. YouTube. URL: https://www.youtube.com/watch?v=FgakZw6K1QQ Retrieved. October 2022

[5] Wikipedia contributors. (2023, January 26). *Principal component analysis*. Wikipedia. URL:https://en.wikipedia.org/wiki/Principal_component_analysis Retrieved. December 2022

[6] *Matrix Theory and Linear Algebra : An open text by Peter Selinger, Based on the original text by Lyryx Learning and Ken Kuttler*, 1st ed. Selinger, P. (2018), Creative Commons License, URL:https://creativecommons.org/licenses/by/4.0/ URL:https://github.com/selinger/linear-algebra

[7] Cheng, C. (2022, September 9). Principal Component Analysis (PCA) Explained Visually with Zero Math. Medium. URL: https://towardsdatascience.com/principal-component-analysis-pca-explained-visually-with-zero-math-1cbf392b9e7d

[8] PCA - CS 357. (n.d.-b). URL: https://courses.grainger.illinois.edu/cs357/fa2022/notes/ref-18-pca.html